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Low-Lying Excitations in the $S = 1$ Antiferromagnetic Heisenberg Chain

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Abstract

In order to confirm the picture of domain-wall excitations in the hidden antiferromagnetic order of the Haldane phase, the structure of the low-lying excitations in the $S = 1$ antiferromagnetic Heisenberg chain is studied by a quantum Monte Carlo method. It is confirmed that there exists a finite energy gap between the first- and the second-excited states at $k = \pi$ as well as between the ground state and the first-excited state at $k = \pi$. In the thermodynamic limit, the second-excited state at $k = \pi$ is separated from the ground state by the gap which is three times as large as the Haldane gap. From the size dependences of the low-lying-excitation energies, the interactions between

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the elementary excitations in the excited states are concluded to be repulsive.

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The structure of low-lying excitations of the $S = 1$ antiferromagnetic Heisenberg chain is one of the main interests in the study on the Haldane system. [1,2] The valence-bond-solid (VBS) model [3,4] introduced by Affleck, Kennedy, Lieb, and Tasaki (AKLT), which gave a clear-cut physical picture of the Haldane massive state, stimulated several authors to study the nature of the excited states. In order to describe the elementary excitations, Knabe [5] considered a triplet bond constructed from two spin-1/2 degrees of freedom in the VBS background, which is now called a crackion, while Arovas, Auerbach, and Haldane [6] discussed a domain wall in the hidden antiferromagnetic order. [7] Later, Fath and Solyom [8] demonstrated that both of the defects have a solitonic nature and actually give the same dispersion relation that well reproduces the elementary excitation spectrum of the AKLT model. [8,9] On the other hand, proposing a new Monte Carlo technique, Takahashi [10] pioneeringly calculated the lower edge of the excitation spectrum as a function of momentum k for the Heisenberg chain. There he further suggested that the lowest excitation of low momentum may be a scattering state of two elementary excitations of momentum $k \sim \pi$. Motivated by his calculation and based on an idea of the hidden domain wall, Gomez-Santos [11] made a variational approach to the Heisenberg chain and showed that the lowest excitations are single-particle-like in the vicinity of $k = \pi$, whereas two-particle-like near $k = 0$. Thus the lower edge of the excitation spectrum has almost fully been investigated so far and it is probable that the elementary excitations are more or less identified with the moving hidden domain wall.

Although nowadays the higher excitation with arbitrary momentum is generally believed to be a scattering state of the elementary domain walls, quantitative investigation of them has not yet been performed well. Developing quite different numerical treatments, White and Huse [12] and the present authors [13] qualitatively pointed out that the lowest excitations as a function of k constitute an isolated band at large k 's, while they coincide with the lower edge of the two-domain-wall continuum at small k 's (Fig. 1). Their suggestion motivates us to calculate the second-lowest excitations. Making use of the Lanczos method, Takahashi [14] calculated $S(q, \omega)$ of the Heisenberg chain of short length as a series of δ -function peaks at

each excited state, which suggests that the lowest excitations are actually separated from the upper continuum at large q 's. For the AKLT model he found that the excitation energy of the second-lowest state at $k = \pi$ is three times as large as one of the lowest state at $k = \pi$. However, the chain length $L \leq 20$ he treated was not long enough to confirm the same scenario in the thermodynamic limit at the Heisenberg point where the correlation length is much longer than that of the AKLT model. Thus the expected multi-domain-wall excitation energies in the thermodynamic limit,

$$E_2(0) - E_G = 2\Delta, \quad E_2(\pi) - E_G = 3\Delta, \quad (1)$$

were not definitely obtained. Here, $E_l(k)$ is the l th eigenvalue in the k -momentum space, $E_G \equiv E_1(0)$ is the ground-state energy, and $\Delta \equiv E_1(\pi) - E_G$ is the Haldane gap.

In order to study the structure of the low-lying energy levels, we exploited an efficient quantum Monte Carlo method. In principle the structure factor $S(q, \omega)$ can be obtained from the spin correlation function along the Trotter axis, $C(\tau)$, which is called the imaginary time correlation function. However, due to an intrinsic difficulty in the numerical treatment of transforming the $C(\tau)$ to $S(q, \omega)$, certain statistical methods such as the maximum-entropy technique, [15–17] have to be introduced for practical calculations at finite temperatures. On the other hand, the lower boundary of the spectrum is simply obtained from a logarithmic plot (log plot) of $C(\tau)$. For the Haldane systems this simple approach works well and a precise value of the lowest state at each momentum has been obtained. [18–21] Let us outline the log-plot method.

We consider a periodic chain of L spins described by the Hamiltonian

$$\mathcal{H} = J \sum_{j=1}^L \mathbf{S}_j \cdot \mathbf{S}_{j+1}; \quad \mathbf{S}_{L+1} = \mathbf{S}_1, \quad (2)$$

where \mathbf{S}_j is the $S = 1$ spin operator. Let us denote the l th eigenvector and eigenvalue of \mathcal{H} in the k -momentum space by $|l; k\rangle$ and $E_l(k)$ [$E_1(k) \leq E_2(k) \leq \dots$], respectively. When the Hamiltonian has the translational symmetry, i.e., $[\mathcal{H}, \mathcal{T}] = 0$,

$$\mathcal{H} |l; k\rangle = E_l(k) |l; k\rangle, \quad \mathcal{T} |l; k\rangle = e^{ik} |l; k\rangle, \quad (3)$$

where \mathcal{T} is the translation operator. The dynamic structure factor in a real frequency domain, $S(q, \omega)$, is the Laplace transformation of the imaginary-time spin correlation function of $S_q^z = L^{-1} \sum_{j=1}^L S_j^z e^{iqj}$:

$$S(q, \tau) = \langle e^{\mathcal{H}\tau} S_q^z e^{-\mathcal{H}\tau} S_{-q}^z \rangle, \quad (4)$$

where $\langle A \rangle \equiv \text{Tr}[e^{-\beta\mathcal{H}} A] / \text{Tr}[e^{-\beta\mathcal{H}}]$ denotes the canonical average at a given temperature $\beta^{-1} = k_B T$. When the system has some conserved quantities, the Hamiltonian is block-diagonalized. Since the total magnetization, $M = \sum_i S_i^z$, is a conserved quantity in the present system, $S(q, \tau)$ is independently defined in each subspace with a given M . Using the complete vector set $|l; k\rangle$ in each subspace, $S(q, \tau)$ is represented as

$$S(q, \tau) = \frac{\sum_{l, l', k} e^{-\beta E_l(k)} |\langle l; k | S_q^z | l'; k + q \rangle|^2 e^{-\tau[E_{l'}(k+q) - E_l(k)]}}{\sum_{l, k} e^{-\beta E_l(k)}}. \quad (5)$$

Thus $S(q, \tau)$ as a function of τ generally exhibits a complicated multi-exponential decay. At a sufficiently low temperature, $S(q, \tau)$ is given as

$$S(q, \tau) = \sum_l |\langle 1; k_0 | S_q^z | l; k_0 + q \rangle|^2 e^{-\tau[E_l(k_0+q) - E_1(k_0)]}, \quad (6)$$

where k_0 is the momentum at which the lowest state in the subspace is located. Now it is reasonable to approximate $E_1(k_0 + q) - E_1(k_0)$ by the slope $-\partial \ln[S(q, \tau)] / \partial \tau$ in the large- τ region satisfying

$$\tau[E_2(k_0 + q) - E_1(k_0 + q)] \gg \ln \frac{|\langle 1; k_0 | S_q^z | n; k_0 + q \rangle|^2}{|\langle 1; k_0 | S_q^z | 1; k_0 + q \rangle|^2}, \quad (7)$$

for an arbitrary n . When the excitations constitute a isolated band and its spectral weight $|\langle 1; k_0 | S_q^z | 1; k_0 + q \rangle|^2$ is large, the inequality (7) is well justified in a wide region of τ . In fact these conditions are satisfied in the Haldane systems. That is why the method did work quite well for the lowest excitations of the present system especially in the large- q region. [18]

Taking a large enough Trotter number, we might, in principle, extract the higher-lying levels from the log plots of $C(\tau)$ for proper regions of τ . However, such an attempt has turned out to be unfeasible with the present numerical facility. Thus we use the log-plot method

for the lowest level at each q , but in the subspaces with various values of M . Combining the calculations in these subspaces, we can construct the low-energy structure and obtain the higher-lying levels. Figure 1 illustrates the probable spectrum of the low-lying states of the system, which is based on the qualitative arguments [12,13] and the calculations for the short chains of $L \leq 20$. [14]

In Fig. 2 we show log plots of $S(q, \tau)$ calculated in the subspaces of $M = 0$, $M = 1$, and $M = 2$ as a function of τ at various values of q , where the lattice constant was set equal to unity. It seems that in general $\ln[S(q, \tau)]$ shows a better linearity at large q 's than at small q 's. We have performed at least a million Monte Carlo steps to obtain $S(q, \tau)$. In most cases the temperature $(\beta J)^{-1}$ and the Trotter number n have been set equal to 0.02 and 200, respectively. We have checked that the thus-obtained data are reliable enough to represent the ground state properties. The numerical precision of the raw data amounts to two digits or more.

As has been mentioned in our previous work, [13] a single spin flip create a domain wall of the hidden order parameter. Thus the lowest-excitation energy is the gap between the lowest singlet state ($S = 0$) and the lowest triplet state ($S = 1$). Because the $S = 0$ state contains a level of $M = 0$, the gap immediately above the ground state is obtained as the energy difference between the two lowest states in the $M = 0$ subspace except for the case of $q = 0$. For $q = 0$, S_q^z commutes with the Hamiltonian and therefore $S(q, \tau)$ does not depend on τ . The excitation energies from the ground state for the $M = 0$ states are obtained as

$$\Delta E_0(q) = \Delta_0(q) \quad (q \neq 0). \quad (8)$$

Here $\Delta E_m(q)$ is the energy difference between the lowest-excited state with a momentum q in the $M = m$ subspace and the ground state, and $\Delta_m(q)$ is the present numerical finding, $-\partial \ln[S(q, \tau)] / \partial \tau$, in the subspace of $M = m$ under the condition (7). Takahashi showed in his recent work [14] that the spectral weight of the lowest excitation at each q is extremely large especially at $q \gtrsim 0.3\pi$ where the lowest excitation is separated from the upper continuum. [11,14] This fact causes the fine linearity of $\ln[S(q, \tau)]$ at large q 's but the less fine

linearity at small q 's, as was observed in Fig. 2(a). In Fact, in our previous attempt [18] to obtain the lower edge of the spectrum, the data at small q 's were not so satisfying as ones at large q 's from the point of the numerical precision. We note that the inelastic-neutron-scattering measurements [23] actually revealed the clear isolated band for the $S = 1$ Haldane material $\text{Ni}(\text{C}_2\text{H}_8\text{N}_2)_2\text{NO}_2(\text{ClO}_4)$.

In the subspace of $M = 1$, the present approach brings us the energy differences between the lowest triplet state ($k = \pi$) and other triplet states with an arbitrary momentum. The excitation energies from the ground state for the $M = 1$ states are obtained as

$$\Delta E_1(q) = \Delta_0(\pi) + \Delta_1(\pi - q). \quad (9)$$

In principle, $\Delta E_0(q)$ obtained from the calculation for $M = 0$ should agree with $\Delta E_1(q)$ obtained from one for $M = 1$. However, a certain difficulty in the present treatment prevents us from reaching the definite coincidence between them. In the $M = 0$ subspace, the lowest state at each q has a relatively large spectral weight, while in the $M = 1$ subspace, this seems not to be the case. Actually, for $M = 1$, the effect of the multi-exponential decay more clearly appears in the log plot of $S(q, \tau)$ especially at small q 's. But, even in the case of $M = 1$, the log plot of $S(q, \tau)$ still gives an almost straight line in the vicinity of $q = \pi$, which results in a precise estimate of $\Delta E_0(0) = \Delta E_1(0) = \Delta_0(\pi) + \Delta_1(\pi)$.

In the subspace of $M = 2$, the present calculation brings us the energy differences between the lowest quintuplet state ($k = 0$) [8] and other quintuplet states with an arbitrary momentum. The excitation energies from the ground state for the $M = 2$ states are obtained as

$$\Delta E_2(q) = \Delta E_0(0) + \Delta_2(q) = \Delta_0(\pi) + \Delta_1(\pi) + \Delta_2(q). \quad (10)$$

Here nonlinearity of $\ln[S(q, \tau)]$ persists in a relatively wide range of τ even at large q 's, which prevents us obtaining a full dispersion curve of the second-excited states.

We plot in Fig. 3 the lowest and the second-lowest eigenvalues, $\Delta E_1(q)$ and $\Delta E_2(q)$, as a function of q for the $L = 64$ chain, which have been obtained using $\Delta_0(\pi)$ and $\Delta_1(\pi)$ at

$L = 64$. Here all the errors arise in estimating the slope of $\ln[S(q, \tau)]$ rather than come from the raw Monte Carlo data. The lowest eigenvalues $\Delta E_1(k)$ were determined, using both of $S(q, \tau)$'s with $M = 0$ and $M = 1$, so as to minimize the numerical ambiguity. Although $\Delta E_2(q)$ has not successfully been obtained in the region of $q \lesssim 0.7\pi$, we here clearly confirm the existence of the isolated band and observe the lower edge of the three-domain-wall continuum as well as one of the two-domain-wall continuum. The overall behavior is almost the same as that for $L = 128$ except in the vicinity of $q = 0$ and $q = \pi$, and therefore we can believe that we are observing the bulk behavior.

In Fig. 4 we show size dependences of the first-excitation energy at the zone boundary, $\Delta E_0(\pi) = \Delta E_1(\pi)$, the first-excitation energy at the zone center, $\Delta E_1(0) = \Delta E_2(0)$, and the second-excitation energy, $\Delta E_2(\pi)$, which are supposed to be the bottom of the single-domain-wall band, one of the two-domain-wall continuum, and one of the three-domain-wall continuum, respectively. Here the symbols \times represent the Takahashi's data [14] for $\Delta E_2(\pi)$ obtained through a different method, which are somewhat inconsistent with our finding beyond the numerical uncertainty. We here observe that the relation (1) comes to hold as L increases. Therefore, we conclude that the low-lying excitations of the present model are regarded as the domain-wall excitations in the hidden antiferromagnetic order.

The chain-length dependences of the energy of the domain-wall-scattering state suggest that there exists a long-range repulsive interaction between the domain walls in the excited states, which is qualitatively consistent with a variational calculation. [24] We note that the interaction between the domain walls is contrastingly attractive in the ground state. [25] In the AKLT model, [14] the relation (1) almost holds even at $L = 16$. It is well known that the spin-spin correlation length is $1/\ln 3 \simeq 0.91$ at the AKLT point, [4] while it is estimated to be 6.2 at the Heisenberg point. [26] Thus the spatial extension of the domain wall is expected to be much larger in the Heisenberg model than in the AKLT model, to which the present significant size dependence is attributed. Smearing the domain wall over three lattice sites, Scharf and Mikeska [9] obtained a variational bound for the Haldane gap of the AKLT model which coincides with the exact-diagonalization result within 1% error. The

spatial extension of the domain wall in the Heisenberg model may reach more than twenty lattice sites.

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FIGURES

FIG. 1. Illustration of the spectrum of the low-lying excited states as a function of momentum for the infinite chain.

FIG. 2. Logarithmic plots of $S(q, \tau)$ versus τ at various values of q for the $L = 64$ chain: (a) $M = 0$, (b) $M = 1$, and (c) $M = 2$.

FIG. 3. The lowest and the second lowest eigenvalues as a function of q for the $L = 64$ chain, where \bigcirc , \diamond , and \square denote the results obtained from $S(q, \tau)$ calculated under $M = 0, 1$, and 2 , respectively.

FIG. 4. Size dependences of the excitation energy of the first-excited state at the zone boundary, $\Delta E_0(\pi)$, one of the first-excited state at the zone center, $\Delta E_1(0)$, and one of the second-excited state at the zone boundary, $\Delta E_2(\pi)$. The black symbols represent the $L \rightarrow \infty$ extrapolated values. The symbols \times represent the Takahashi's calculations [14] for $\Delta E_2(\pi)$ obtained with an exact-diagonalization technique.

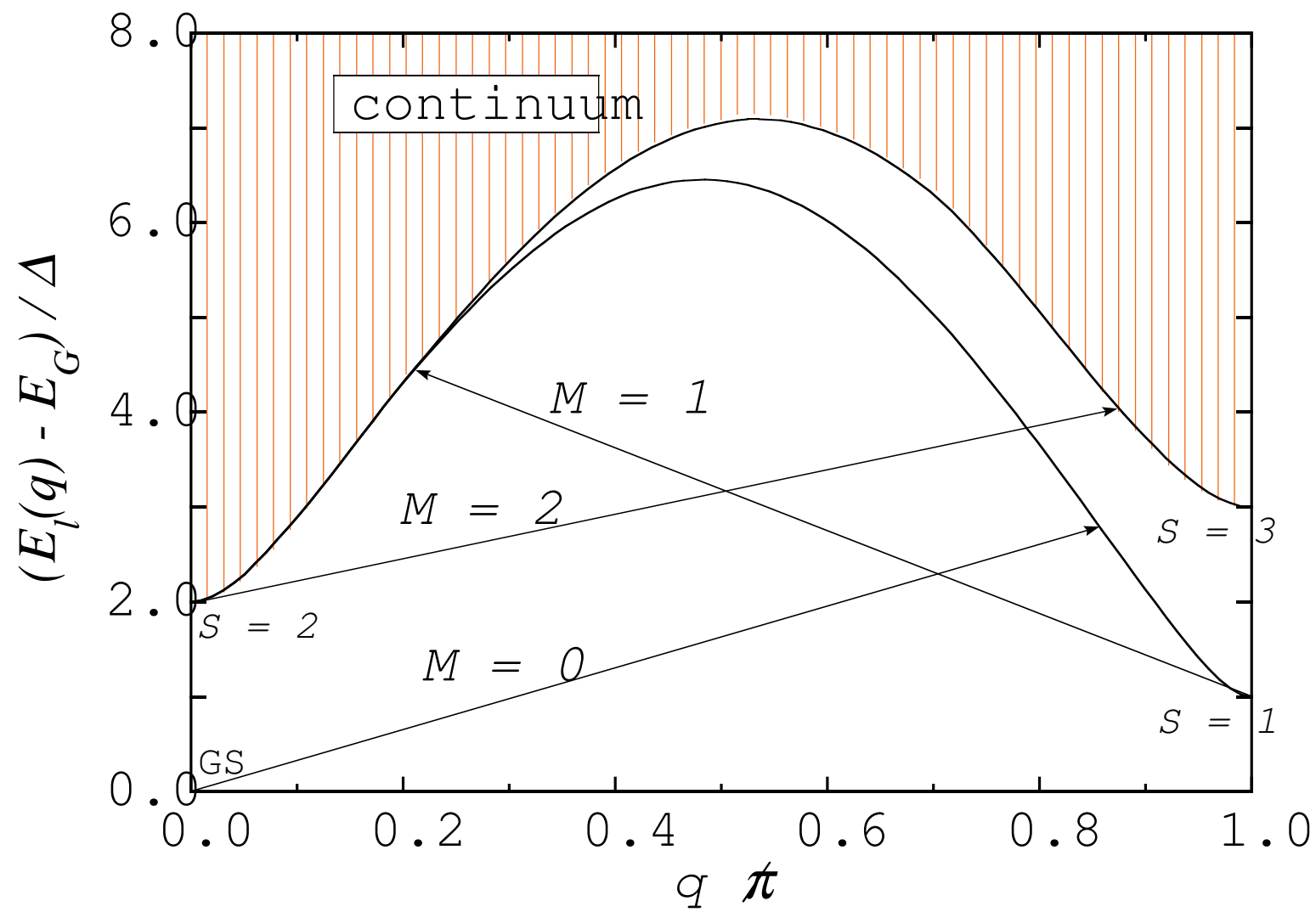


Fig. 1 S. Yamamoto et al.

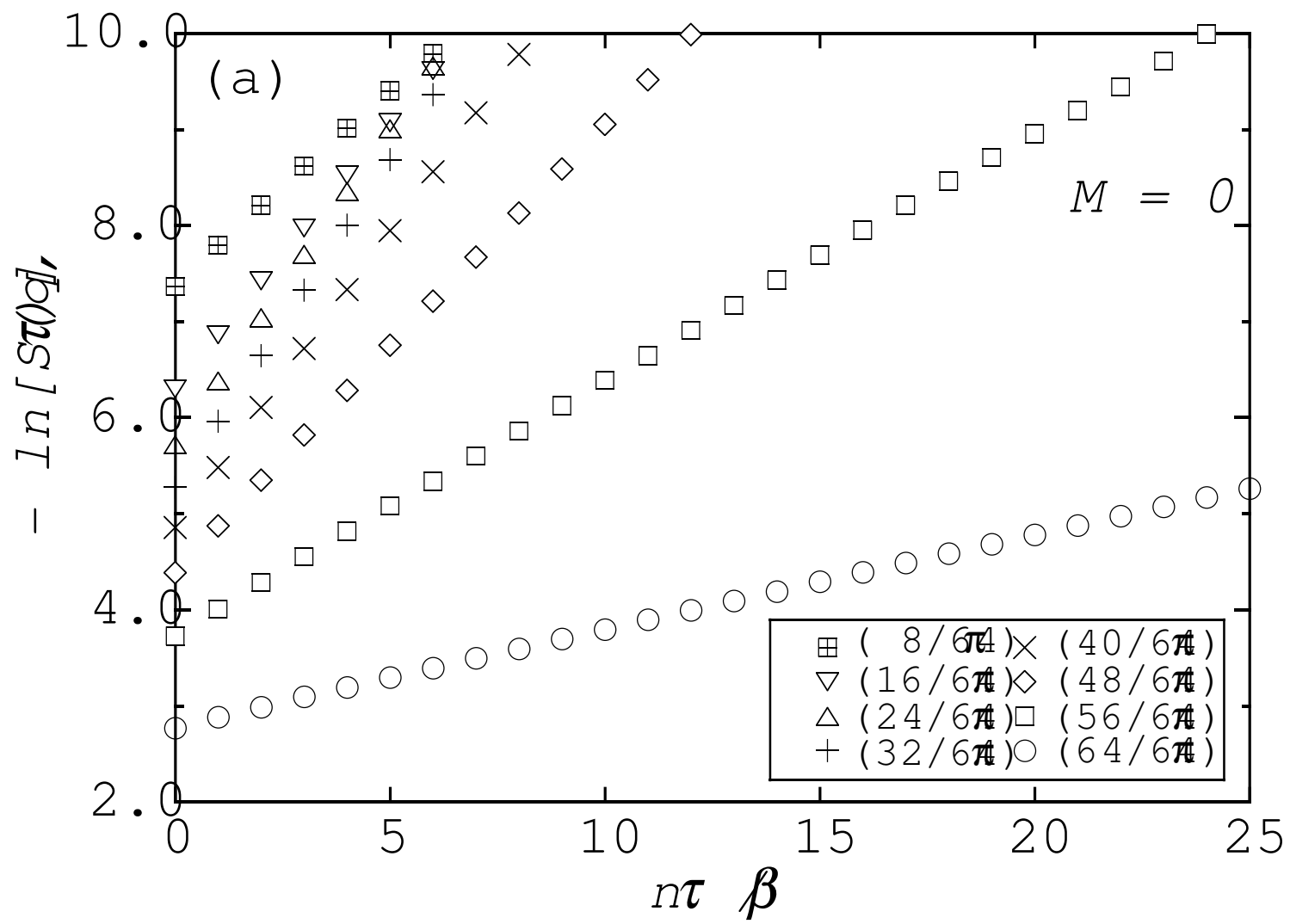


Fig. 2(a) S. Yamamoto et al.

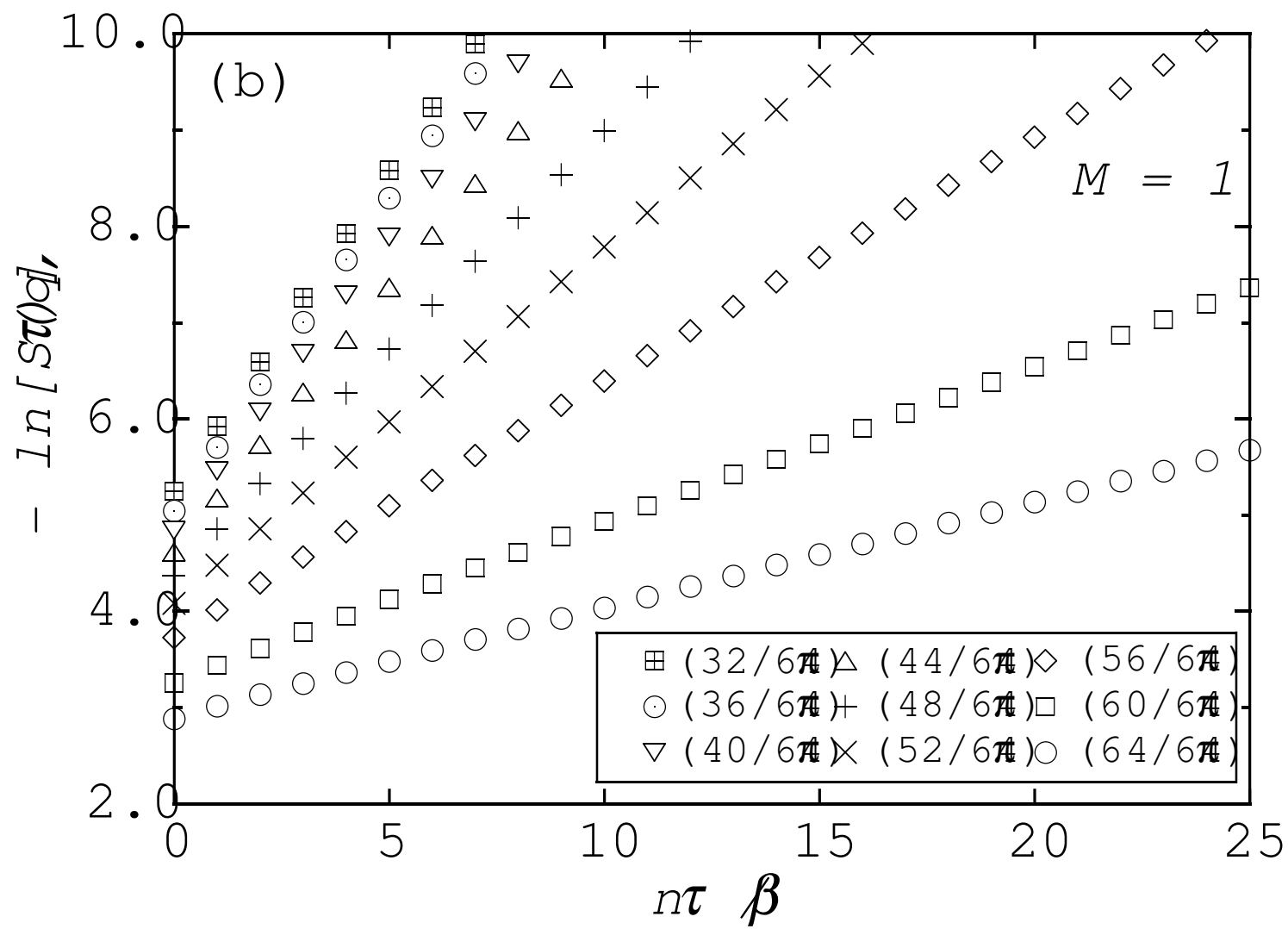


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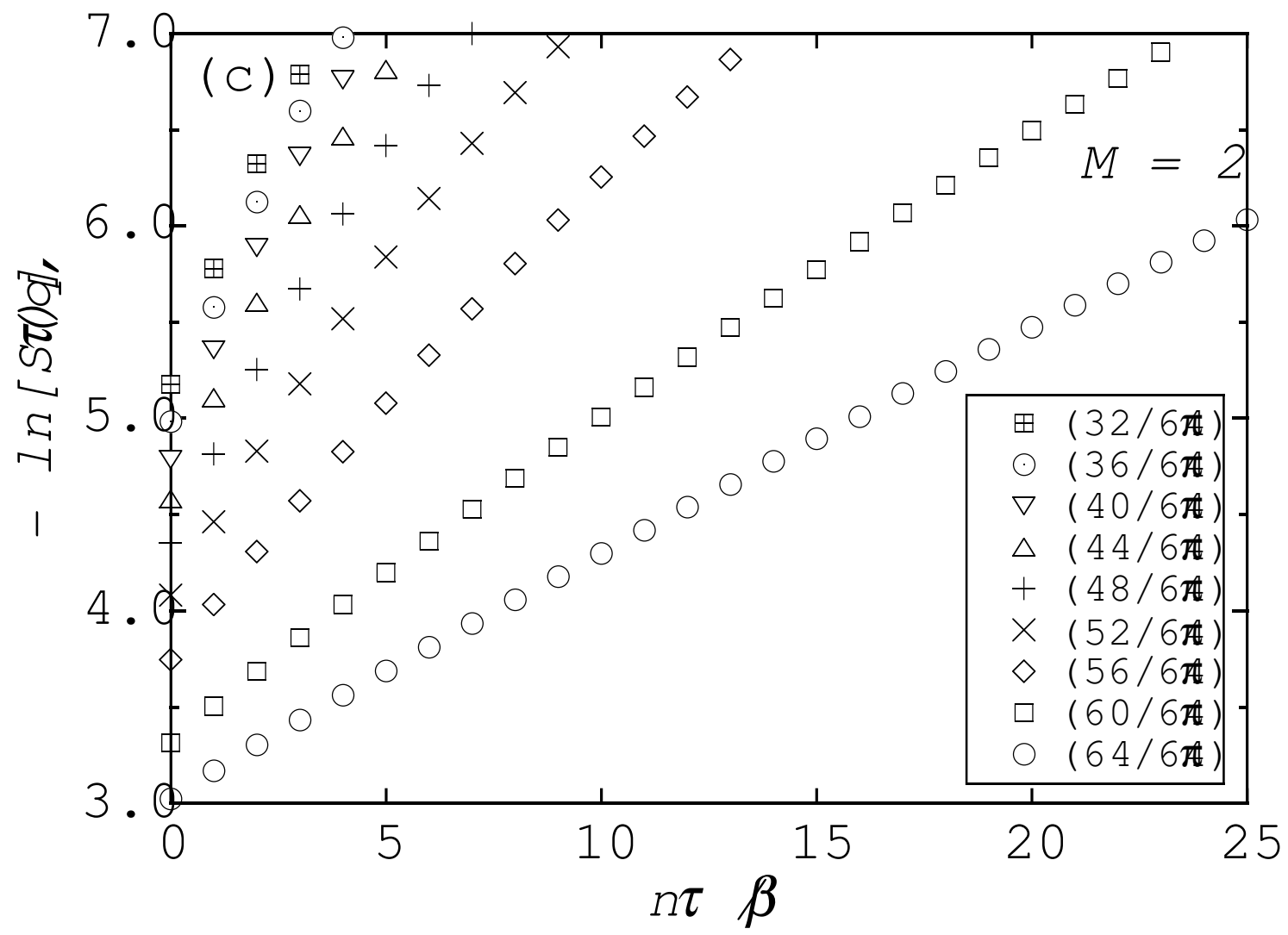


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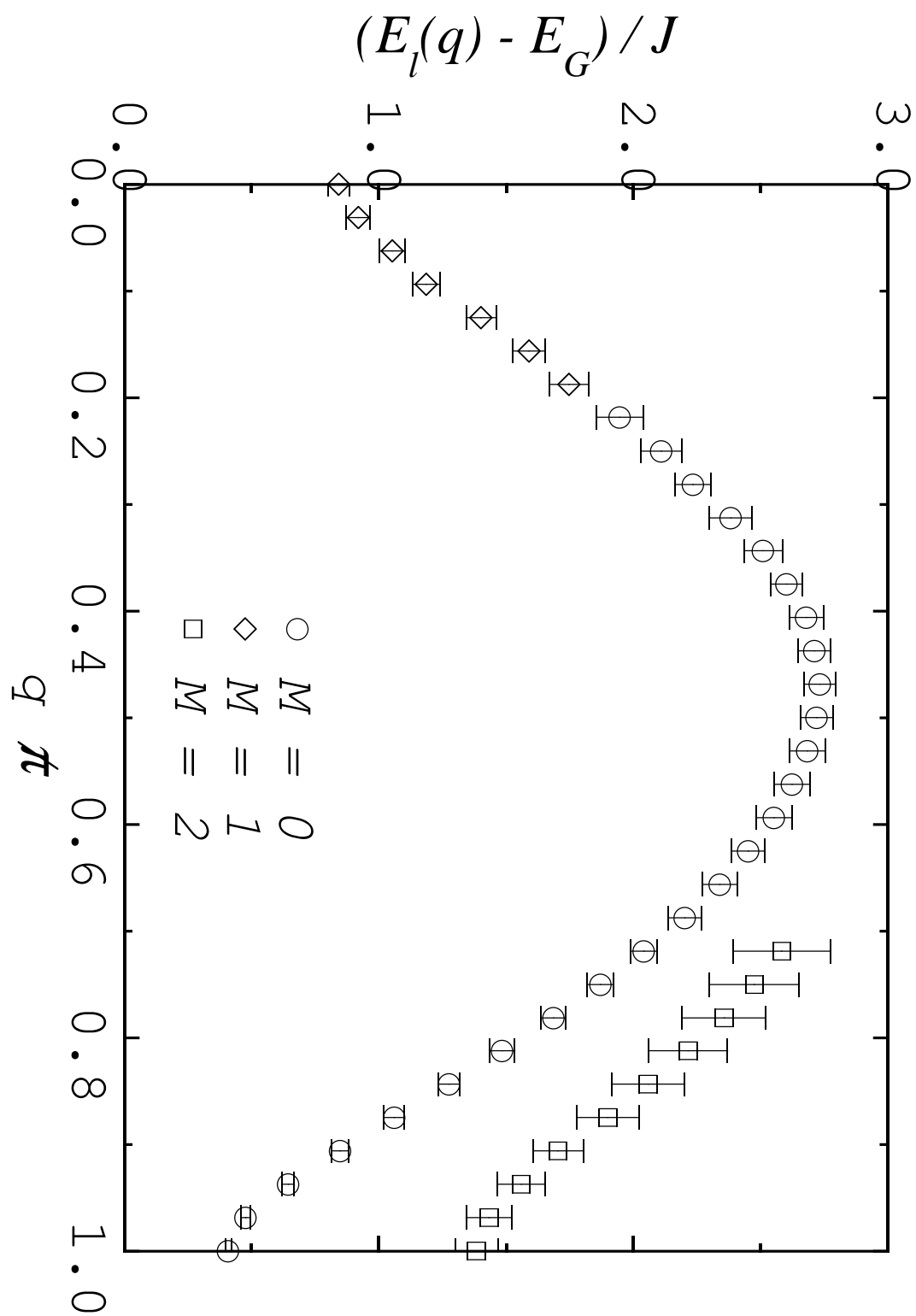


Fig. 3 S. Yamamoto et al.

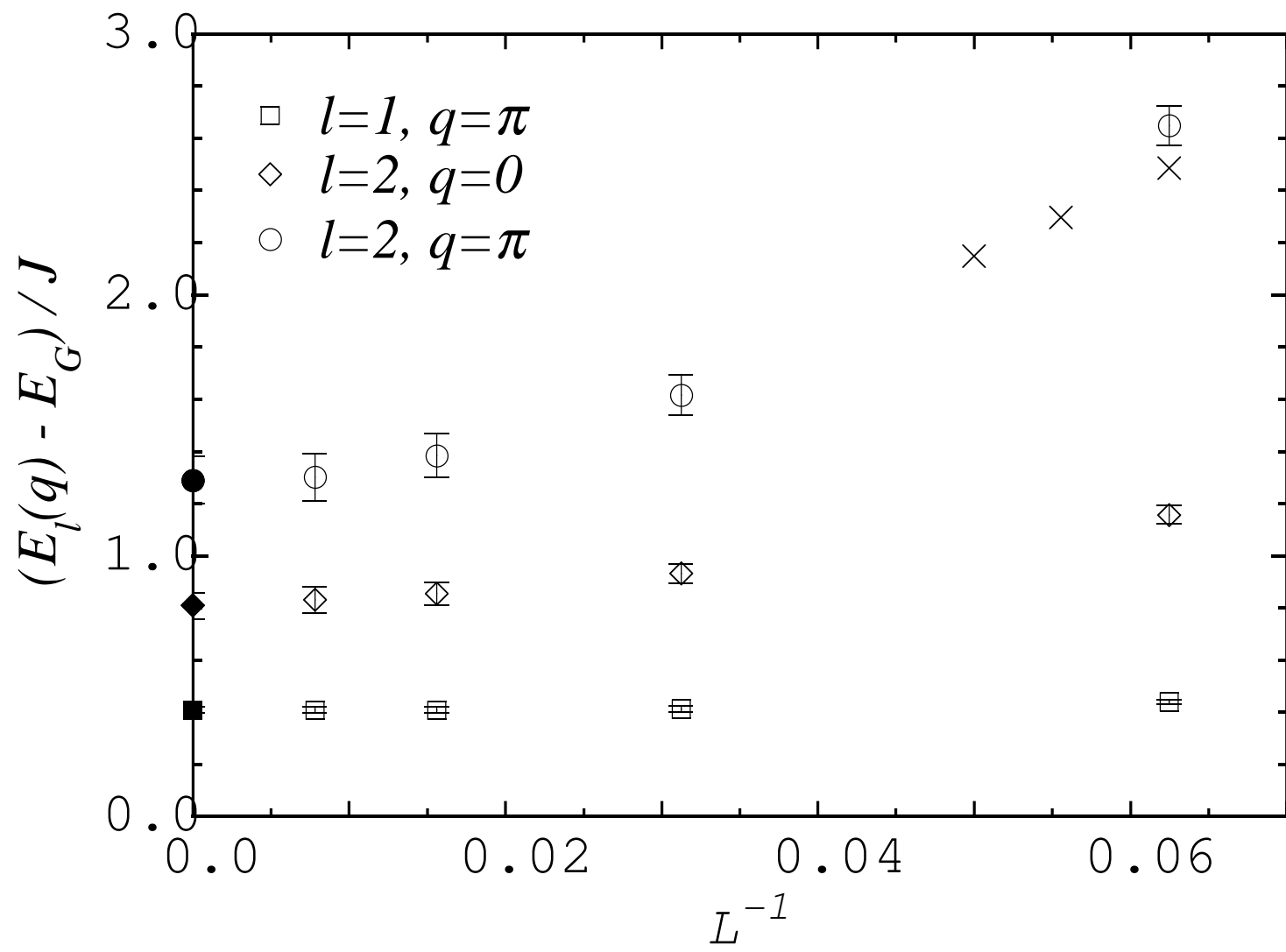


Fig. 4 S. Yamamoto et al.